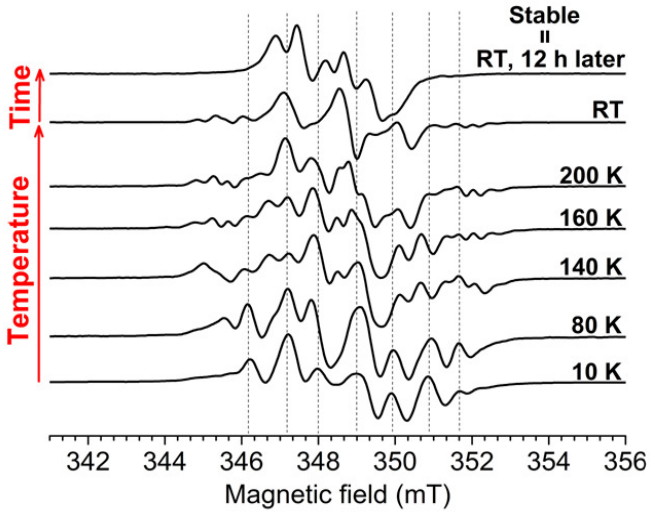
Thermally activated reactions of radiation-induced radicals in sugar single crystals: an electron magnetic resonance and DFT study, H. De Cooman, H. Vrielinck, E. Pauwels, E. Sagstuen, M. Waroquier, F. Callens, *7th European Federation of EPR (EFEPR) Groups Meeting and Closing Meeting of COST P15*, Antwerp, Belgium, **6 - 11 September 2009**

Radiation-induced radicals *in solid sugars* are studied (i) as model systems to gain insight into the radiation chemistry of the DNA deoxyribose unit and (ii) because of their potential as (emergency) dosimeters. Electron magnetic resonance (EMR) measurements allow for a detailed characterisation of such radicals via their (proton) hyperfine and ***g*** tensors. Theoretical calculations of these tensors with density functional theory (DFT) codes provide an excellent tool to help analyse and interpret experimental results.
X-irradiation typically induces several primary radicals in solid sugar systems, which transform into stable radicals or diamagnetic species via one or more thermally driven radical reactions. The primary and intermediate radical species can be studied by EMR measurements after *in-situ* irradiation at low temperature.
Recently we have identified, using a combined EMR and DFT approach, the structure of the major radiation-induced stable radicals in solid sucrose[1,2,3], and we are currently investigating their formation mechanism by *in-situ* EMR measurements at 10 K, 80 K and 140 K, annealing experiments after irradiation at 10 K (see figure, for B // <c*>) and DFT modeling. An overview of the results obtained so far will be presented.



References

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